REMARKS/ARGUMENTS

The office action issued October 17, 2006 continues the rejection of claim 1 under 35 U.S.C. § 102(b). In addition, a new rejection under 35 U.S.C. § 101 has been applied to claim 1. Claims 2-7, which were previously allowed, are now rejected under 35 U.S.C. § 101 but "...would be allowable if rewritten including all of the limitations of the base claim and any intervening claims, and to overcome the above rejection."

35 U.S.C. 102(b)

Examiner's Rejection:

The Examiner has continued the rejection claim 1 under 35 U.S.C. 102(b): "... as being anticipated by International Application Publication Number WO 99/44055 to Nicholls." Specifically, the Examiner states:

> With regard to claim 1 Nicholls discloses a computer implemented method to search a heterogeneous compound database composed of molecules from different sources and syntheses, some known and some unknown, for molecules which have the same biological activity as a known query molecule (see abstract) comprising the steps of fragmenting a query molecule and a database molecule according to a defined set of rules (see page 10 line 25), generating shape descriptors for the query molecule and database molecule fragments (see page 22 line 10-19), and using the shape descriptors identifying the database molecule which has a shape similar to the query molecule (see page 25 line 5-26).

Applicants' Response:

Applicant have previously responded to the 35 U.S.C. § 102(b) rejection by discussing aspects of the Nicholls' disclosure that Applicants believed were not appreciated by the Examiner. However, Applicants' arguments have not been found persuasive by the Examiner. For purposes of the present Response, Applicants will concede arguendo that the Examiner is correct that Nicholls teaches:

1) fragmenting a query molecule and a database molecule according to a defined set of rules (see page 10 line 25)

2) generating shape descriptors for the query molecule and database molecule fragments (see page 22 line 10-19); and

3) using the shape descriptors identifying the database molecule which has a shape similar to the query molecule (see page 25 line 5-26).

It is Applicant's position, however, that the Examiner credits the disclosure with more information than is in it. In particular, Nicholls discloses using his descriptor of whole molecules to find shape similar molecules but gives no indication of how he would use descriptors of the fragments to find similarly shaped whole molecules. Nicholls does speak to forming descriptors of what he calls fragments, but other than an allusion that searching methods similar to those he described with respect to whole molecule searching could be used with fragments, Nicholls provides no specific teaching. The whole molecule searching method does not teach how to take multiple fragments into account.

Applicants, on the other hand, describe very specific methods to identify the most similarly shaped molecule in the database. Applicants compare each query fragment with each database molecule fragment as fully set forth in the specification beginning on page 16. Further, Applicants on pages 18 – 24 teach searching using two and three piece fragmentations as well as subset searching and core searching. Finally, Applicants teach the use of features in conjunction with shape searching. Even conceding arguendo that Nicholls teaches what is set forth in items 1-3 above, Nicholls does not teach the fragment comparison methods described in detail by Applicants. Applicants have amended claim 1 to more set forth that which they claim is their invention with particular reference to the query and database molecule comparisons. In view of the amendment and the argument presented, Applicants respectfully submit that Nicholls does not anticipate Applicants' invention and request the Examiner to withdraw the 35 U.S.C. § 102(b) rejection.

35 U.S.C. § 101

Examiner's Rejection:

The Examiner has rejected claims 1-7 under 35 U.S.C. 101 as being directed to non-statutory subject matter, specifically stating that "The claims merely recite an algorithm for manipulating data in a computer and no tangible result, such as a display, is produced."

Applicants' Response:

The rationale for the Patent Office reintroducing this line of rejection is unclear to Applicant's attorney since claims of the type presented in the case have long been found to be

statutory (as, for instance, were claims 2-7 under the prior office interpretation before the most recent action) without the need to put Applicants to the burden of demonstrating that the invention as claimed is concrete, tangible, and useful. Be that as it may, Applicants understand that the Examiner is bound by the latest Office interpretation and will respond accordingly.

Applicants respectfully submit that the invention is more than a "mere algorithm" and that it produces a meaningful real world result very useful in the medicinal arts. Applicants will respond to each of the three criteria discussed in the USPTO Internet web reference cited by the Examiner. As noted, USEFULL in the context of the USPTO's interpretation of the utility requirement means that the utility of an invention has to be (i) specific, (ii) substantial and (iii) credible. The method of the present invention permits questions to be asked and answered that could not have previously been considered. In particular, modern biochemistry recognizes the importance of 3D molecular shape as a principal feature of biochemical interactions. Given a lead compound, the question can be posed: what other molecules have the same three dimensional shape as the known molecule? In pharmacological research, large libraries of synthesized or discovered compounds exit. They may have been prepared as a result of attempts to increase the activity or specificity of a particular line of compounds or they might have resulted from screening soil samples or they might have been prepared as general searching libraries. Whatever led to their formation, the result is that the databases of such libraries hold many molecules that are likely to have applications outside of a specific area.

Until the present invention, there was no way to search such molecular libraries for compounds that had similar 3D shape to a query molecule by fragmenting the query and database molecule into fragments and determing, on the basis of fragment to fragment similarity, which database molecule was sufficiently similar in 3D shape to the query molecule. Using the present invention, the various libraries of available compounds can be searched for shape similar compounds. This process clearly yields specific, substantial, and credible results since specific molecules having specific attributes are identified. Applicants submit that the "Useful" criteria are fully met.

TANGIBLE means that the claim must set forth an implementation to produce a real-world result. The identification of molecules that will have the same three dimensional shape and likely biological activity of a query molecule (typically a lead compound) is a tangible result. It is not abstract. The fact that the molecule is identified by a computer implemented method does not make the identification abstract. It is tied to a specific characterized molecular characteristic, namely three dimensional shape. Applicants respectfully submit that the "Tangible" criteria is fully met.

"CONCRETE" requires that there be predictability to the invention. That is certainly the case here. The fragments from both the query molecule and the database molecule are characterized with the same methodology employing a validated metric. The metric characterization of the fragments does not vary from time to time. The calculated similarity (or dissimilarity) distance does not vary from time to time. Accordingly, the same query molecule

used to search the same database library will always yield the same results. Applicants respectfully submit that the "Concrete" criteria is fully met.

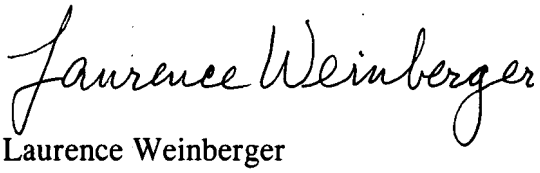
There is the suggestion in the Examiner's comments that some form of specific output is required for there to be a tangible result. Under the analysis of "tangible" presented above, Applicants do not think that this is necessary under the law as currently interpreted by the courts. However, clearly the results of the application of the present method are communicated to the real world user through an output as discussed in the specification. The output code supplied with the application, among other characteristics, provides query and database molecule structural identification, fragment identification, and degree of similarity measures. Applicants have amended the claims to recite output of the results provided by the method of the invention. In addition, new dependent claims are presented directed to the output. Antecedent basis for the amendments and new claims is found on page 29 of the specification.

Finally, Applicants do not believe, given the amendments and arguments presented herein, that it is necessary to rewrite claims 2-7 in dependent form. The claims have been amended to correct the spelling of heterogeneous. While several additional new claims have been added by amendment, no additional fees are due since the total number of independent and dependent claims is still less than twenty.

In view of the claim amendments and the arguments presented above, Applicants respectfully request the Examiner to withdraw all rejections and pass the application to issue.

April 17, 2007

Respectfully submitted,



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